Higher-order numerical integration using subtraction terms

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1. General procedure
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3. Two-loop examples
4. Public code NICODEMOS

General procdure

Challenges for numerical loop integrations:

1. Isolation of UV and IR singularities
2. Stable convergence, in particular when integrating over thresholds

1. Suitable subtraction terms, which can be integrated analytically

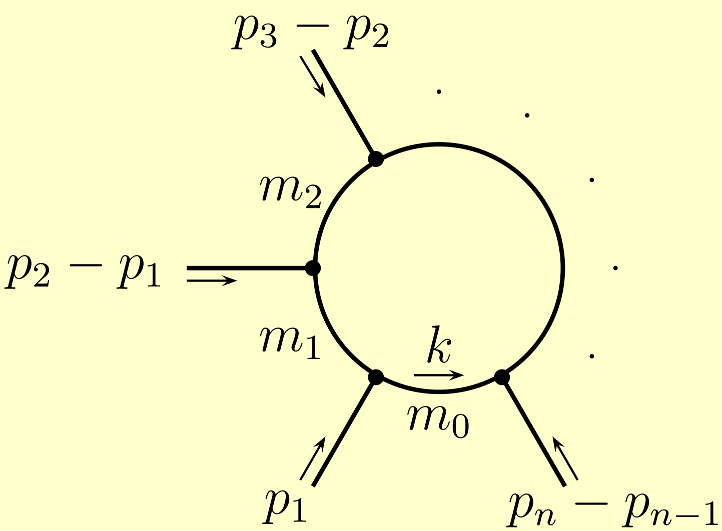
   Nagy, Soper '03

   Becker, Reuschle, Weinzierl '10

2. Complex deformation of integration contour — Nagy, Soper '06

   Anastasiou, Beerli, Daleo '07

IR subtraction



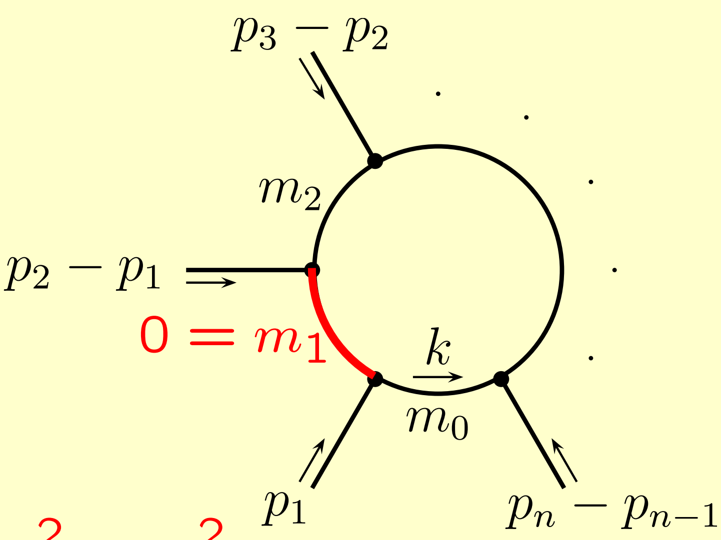
$$I^{(1)} = \int \widetilde{dk}\, \frac{N(k)}{D^{(1)}(k)}$$

$$\widetilde{dk} = e^{\gamma_E (4-d)/2} \frac{d^d k}{i\pi^{d/2}}$$

$$D^{(1)}(k) = [k^2 - m_0^2][(k-p_1)^2 - m_1^2] \cdots [(k-p_n)^2 - m_n^2]$$

IR subtraction

Soft singularity:



$p_1^2 = m_0^2$

$(p_2 - p_1)^2 = m_2^2$

$$I^{(1)} = \int \widetilde{dk} \, \frac{N(k)}{D^{(1)}(k)}$$

$$\widetilde{dk} = e^{\gamma_E (4-d)/2} \frac{d^d k}{i\pi^{d/2}}$$

$$D^{(1)}(k) = [k^2 - m_0^2][(k-p_1)^2 - m_1^2] \cdots [(k-p_n)^2 - m_n^2]$$

$$G^{(1)}_{\text{soft}} = \frac{N(k{=}p_1)}{[k^2 - m_0^2][(k-p_1)^2][(k-p_2)^2 - m_2^2]} \prod_{j \neq 0,1,2} \frac{1}{(p_1 - p_j)^2 - m_j^2}$$

Becker, Reuschle, Weinzierl '10

$$I^{(1)}_{\text{reg}} = \int \widetilde{dk} \left(\frac{N(k)}{D^{(1)}(k)} - G^{(1)}_{\text{soft}} \right)$$

IR subtraction

Integrated soft subtraction term:

$m_0 = m_2 = 0$:
$$\int \widetilde{dk}\, G^{(1)}_{\text{soft}} = F_{\text{rem}}\, \frac{1}{s}\left[\frac{1}{\varepsilon^2} - \frac{1}{\varepsilon}\log(-s) + \frac{\log^2(-s)}{2} - \frac{\pi^2}{12}\right],$$

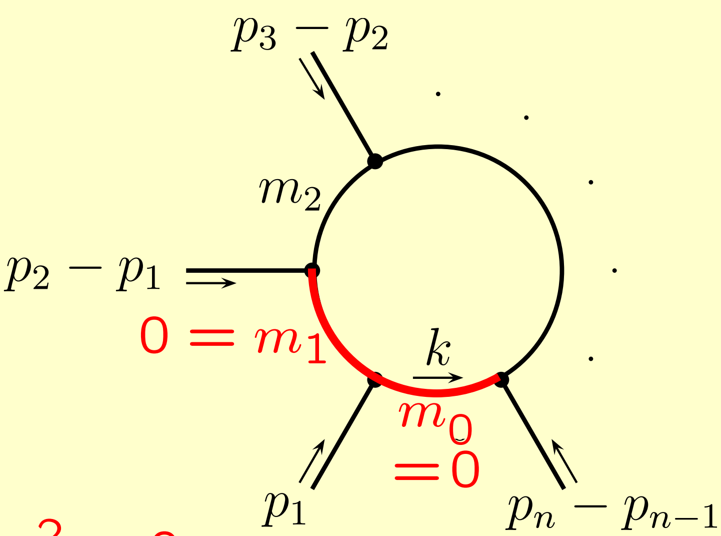
$m_0 > 0$, $m_2 = 0$:
$$\int \widetilde{dk}\, G^{(1)}_{\text{soft}} = F_{\text{rem}}\, \frac{1}{s - m_0^2}\left[\frac{1}{2\varepsilon^2} - \frac{1}{\varepsilon}\log\left(\frac{m_0^2 - s}{m_0}\right) + \frac{\pi^2}{24} + \frac{\log^2(m_0^2 - s)}{2} - \log^2(m_0) - \text{Li}_2\left(\frac{-s}{m_0^2 - s}\right)\right],$$

$$F_{\text{rem}} = N(k{=}p_i) \prod_{\substack{j\neq \\ i-1,\, i,\, i+1}} \frac{1}{(p_i - p_j)^2 - m_j^2}$$

$$\varepsilon = (4-d)/2, \qquad s = (p_{i+1} - p_{i-1})^2 + i\epsilon$$

IR subtraction

Collinear singularity:



$p_1^2 = 0$

$$I^{(1)} = \int \widetilde{dk}\, \frac{N(k)}{D^{(1)}(k)}$$

$$\widetilde{dk} = e^{\gamma_{\mathsf{E}}(4-d)/2} \frac{d^d k}{i\pi^{d/2}}$$

$$D^{(1)}(k) = [k^2 - m_0^2][(k-p_1)^2 - m_1^2] \cdots [(k-p_n)^2 - m_n^2]$$

$$G^{(1)}_{\mathsf{coll}} = \frac{N(k{=}p_1)}{k^2(k-p_1)^2} \prod_{j \neq 0,1} \frac{1}{(p_1 - p_j)^2 - m_j^2}$$

$$\int \widetilde{dk}\, G^{(1)}_{\mathsf{coll}} = 0$$

$$I^{(1)}_{\mathsf{reg}} = \int \widetilde{dk} \left(\frac{N(k)}{D^{(1)}(k)} - G^{(1)}_{\mathsf{coll}} \right)$$

Variable mapping

- After IR subtraction:

$$I^{(1)}_{\text{reg}} \equiv I^{(1)} - \sum \int \widetilde{dk}\, G^{(1)}_{\text{soft}} - \sum \int \widetilde{dk}\, G^{(1)}_{\text{coll}} = \int \widetilde{dk}\, \frac{N_{\text{reg}}(k)}{D^{(1)}(k)}$$

- Introduce Feynman parameters and map onto hypercube:

$$I^{(1)}_{\text{reg}} = \int_0^1 dy_1 \ldots dy_n \int \widetilde{dk}\, \frac{\tilde{N}(k)}{[k^2 - A]^n}$$

- Tensor reduction:

$$\int \widetilde{dk}\, \frac{k^{\mu_1} k^{\mu_2} \ldots k^{\mu_r}}{[k^2 - A]^n}$$

$$= \frac{1}{r!!\, d(d+2) \cdots (d+r-2)} \sum_{\text{permut.}} (g^{\mu_1\mu_2} \ldots g^{\mu_{r-1}\mu_r}) \int \widetilde{dk}\, \frac{k^r}{[k^2 - A]^n}$$

Variable mapping

- Integration over k and expansion in ε:

$$I^{(1)}_{\text{reg}} = \int_0^1 dy_1 \dots dy_{n-1} \Big[\underbrace{D_0 \Big(\frac{1}{\varepsilon}}_{\text{UV poles}} + \log(A - i\epsilon) \Big) + D_1 (A - i\epsilon)^{-1} + D_2 (A - i\epsilon)^{-2} + \dots \Big]$$

- Physical thresholds: A changes sign in ingration region
  $\longrightarrow$ Problematic for numerical integrators

  $\longrightarrow$ Deform Feynman parameter integration into complex plane:

Nagy, Soper '06

$$y_i = z_i - i\lambda z_i (1 - z_i) \frac{\partial A}{\partial z_i}, \qquad 0 \leq z_i \leq 1.$$

$$A(\vec{y}) = A(\vec{z}) - i\lambda \sum_i z_i (1 - z_i) \Big(\frac{\partial A}{\partial z_i} \Big)^2 + \mathcal{O}(\lambda^2).$$

Typical choice: $\lambda \sim 0.5\text{--}1$

Numerical integration

Finite, non-singular numerical integral, for each order in ε:

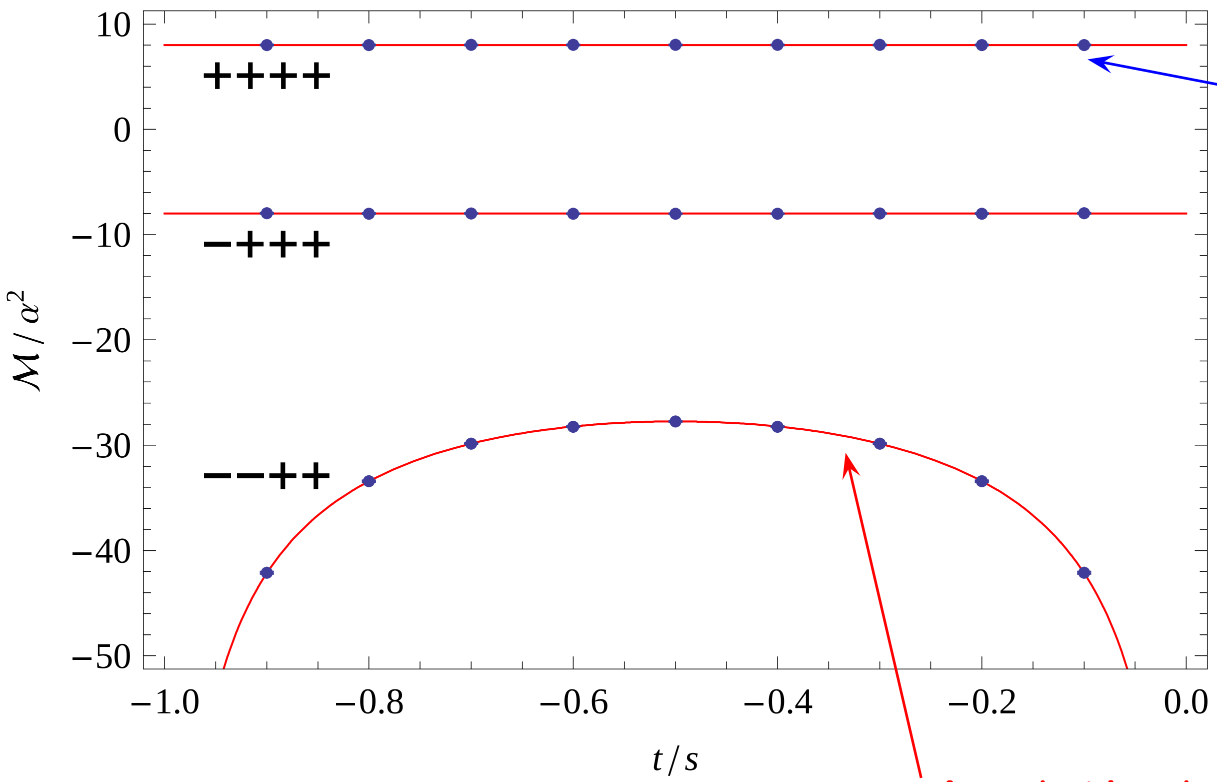
$$I_{\text{reg}}^{(1)} = \int_0^1 dz_1 \ldots dz_{n-1} \left| \frac{\partial(y_1, \ldots, y_{n-1})}{\partial(z_1, \ldots, z_{n-1})} \right| \left[D_0 \left(\frac{1}{\varepsilon} + \log(A - i\epsilon) \right) \right.$$
$$\left. + D_1 A^{-1} + D_2 A^{-2} + \ldots \right]$$

Use CUBA package, integration routines VEGAS and CUHRE

Hahn '05

One-loop examples

$\gamma\gamma \to \gamma\gamma$: (no UV/IR singularities)



Numerical integration (with error bars)

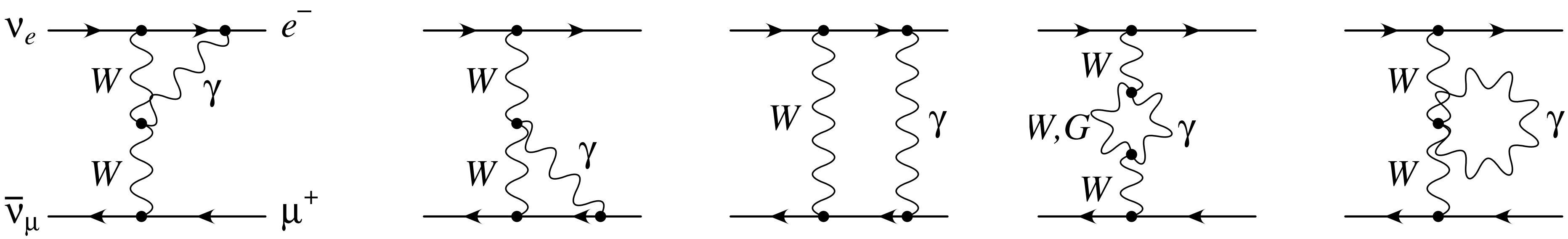
Analytical result

VEGAS routine,
$N = 3 \times 10^6$,
$\lambda = 1$

Binoth, Glover, Marquard, v.d.Bij '02

One-loop examples

$\nu_e \bar{\nu}_\mu \to e^- \mu^+$: (UV, soft, and collinear singularities)



	numerical	analytical
$\mathcal{O}(\varepsilon^{-2})$	-0.625	-0.625
$\mathcal{O}(\varepsilon^{-1})$	1.1311336(5)	1.131133655
$\mathcal{O}(\varepsilon^{0})$	3.27791(4)	3.277923432

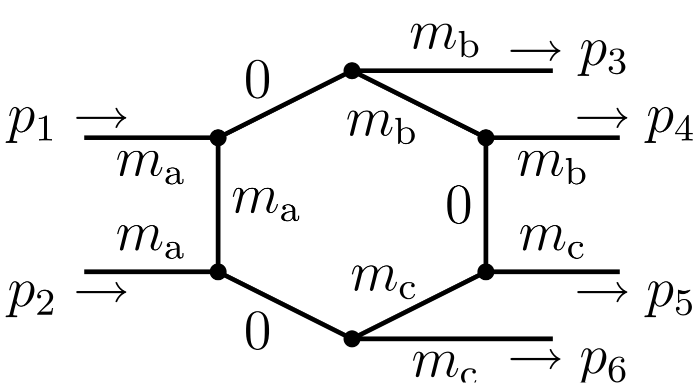
$M_\mathrm{W} = 1,\ s = 2,\ t = -1$

using CUHRE routine,
$N = 5 \times 10^5$, $\lambda = 0.5$

using PV reduction and
basic A_0, B_0, C_0, D_0 functions

One-loop examples

Scalar hexagon (with soft singularities)



CUHRE routine, $N = 10^7$, $\lambda = 0.5$

$\mathcal{O}(\varepsilon^{-1})$: $-\,0.0044718804 + 0.0120697975i$

$\mathcal{O}(\varepsilon^{0})$: $-\,0.04383(14) - 0.00790(14)i$

$$m_\mathrm{a}^2 = 1.0, \quad \vec{p}_1 = (0,0,3), \quad \vec{p}_2 = (0,0,-3),$$
$$m_\mathrm{b}^2 = 0.25, \quad \vec{p}_3 = (0.5,0,0.5), \quad \vec{p}_4 = (-0.2,0,0.1),$$
$$m_\mathrm{c}^2 = 4.0, \quad \vec{p}_5 = (0,1.37626,-0.3), \quad \vec{p}_6 = (-0.3,-1.37626,-0.3)$$

Extension to two loops

- **UV divergencies:** in either or both *subloops*, and also *global*

  $\longrightarrow$ Direct evaluation not possible, need **UV subtraction terms**

  $\longrightarrow$ UV singularities in both subloops only for tadpoles & selfenergies, not considered here

- **IR divergencies:** in either or both *subloops*, also overlapping

  $\longrightarrow$ Here: only consider IR singularity in one loop, other cases left for future work

General form of two-loop integral:

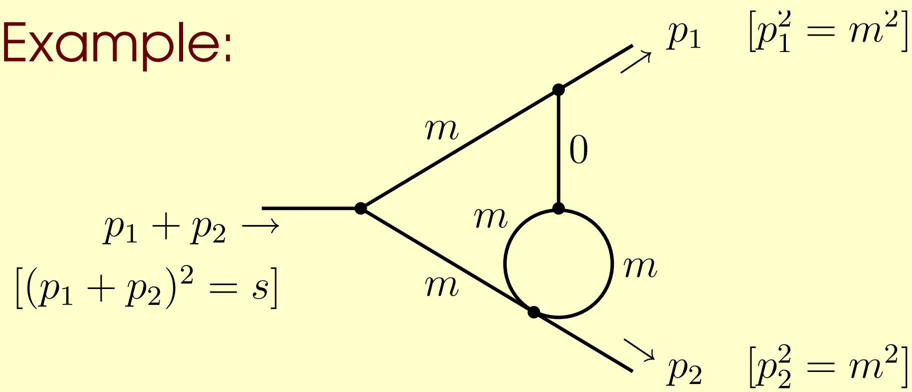
$$I^{(2)} = \int \widetilde{dk}_1 \widetilde{dk}_2 \, \frac{N(k_1,k_2)}{D^{(2)}(k_1,k_2)}$$

$$\begin{aligned} D^{(2)}(k_1,k_2) = {} & [k_1^2 - m_0^2][(k_1-p_1)^2 - m_1^2]\cdots[(k_1-p_r)^2 - m_r^2] \\ & \times [(k_2-p_{r+1})^2 - m_{r+1}^2]\cdots[(k_2-p_s)^2 - m_s^2] \\ & \times [(k_1-k_2-p_{s+1})^2 - m_{s+1}^2]\cdots[(k_1-k_2-p_n)^2 - m_n^2] \end{aligned}$$

Subloop IR divergencies

Subtraction procedure as for one-loop case

Example:



$$I_5 = \int \widetilde{dk}_1 \widetilde{dk}_2 \; \frac{1}{[k_1 - m^2][(k_1 - p_1)^2][(k_1 - p_1 - p_2)^2 - m^2]} \times \frac{1}{[(k_2 - p_1)^2 - m^2][(k_1 - k_2)^2 - m^2]}$$

Soft subtraction term:

$$G^5_{\text{soft}} = \frac{1}{[k_1 - m^2][(k_1 - p_1)^2][(k_1 - p_1 - p_2)^2 - m^2]} \times \frac{1}{[(k_2 - p_1)^2 - m^2][(p_1 - k_2)^2 - m^2]}$$

Two-loop UV divergencies

Global UV divergency:

$$G^{(2)}_{\text{glob}} = \left. \frac{N(k_1, k_2)}{D^{(2)}(k_1, k_2)} \right|_{p_i = 0}$$

Works for all two-loop N-point functions except selfenergies

$\int \widetilde{dk}_1 \widetilde{dk}_2 \, G^{(2)}_{\text{glob}}$ consists of two-loop vacuum integrals

$\longrightarrow$ known analytically Davydychev, Tausk '92

$I^{(2)}_{\text{gs}} \equiv I^{(2)}_{\text{reg}} - \int \widetilde{dk}_1 \widetilde{dk}_2 \, G^{(2)}_{\text{glob}}$ can have singularities in one subloop

(both subloops only for tadpoles and selfenergies)

Two-loop UV divergencies

Subloop UV divergency in k_1 loop:

- Introduce Feynman parameters for k_1 subloop and perform k_1 tensor reduction (as before)

contain all k_2 dependence

$$I_{\text{gs}}^{(2)} = \int_0^1 dy_1 ... dy_{m-1} \int \widetilde{dk_1}\widetilde{dk_2} \left[\frac{C_1}{[k_1^2 - A]^m} + \frac{C_2}{[k_1^2 - A]^{m-1}} + \dots \frac{C_j}{[k_1^2 - A]^2}\right],$$

of k_1 propagators

UV diverg.

- UV subloop subtraction term:

$$G_{\text{sub}}^{(2)} = \int_0^1 dy_1 \dots dy_{m-1} \frac{C_j}{[k_1^2 - \mu^2]^2},$$

($\mu =$ suitably chosen mass parameter)

Two-loop UV divergencies

Subloop UV divergency in k_1 loop:

- Integrated subtraction term:

$$\int \widetilde{dk}_1 \widetilde{dk}_2\, G^{(2)}_{\mathrm{sub}} = -\Gamma(\varepsilon - 2)\mu^{2-\varepsilon} \int_0^1 dy_1 \dots dy_{m-1} \underbrace{\int \widetilde{dk}_2\, C_j}_{\substack{\text{one-loop integral} \\ \text{(same procedure as above)}}}.$$

- Remainder $I^{(2)}_{\mathrm{rem}} \equiv I^{(2)}_{\mathrm{reg}} - \int \widetilde{dk}_1 \widetilde{dk}_2\, G^{(2)}_{\mathrm{glob}} - \int \widetilde{dk}_1 \widetilde{dk}_2\, G^{(2)}_{\mathrm{sub}}$ is finite

- Feynman parameters for k_2 subloop

- Tensor reduction for k_2 terms

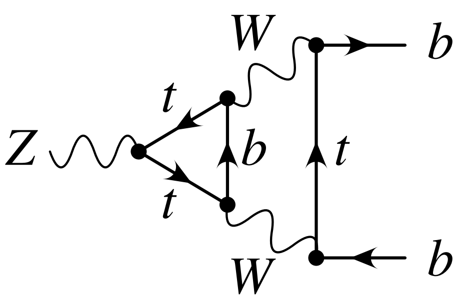
- Perform k_1 and k_2 integrals
  $\longrightarrow$ Numerical integral over Feynman parameters

- Deform integration contour as necessary

Two-loop examples

Diagram contributing to $Z \to b\bar{b}$:

(global and subloop UV singularities, no IR singularity)



	this work	BT method*
$\mathcal{O}(\varepsilon^{-2})$	−2.30183413	−2.30183413
$\mathcal{O}(\varepsilon^{-1})$	5.07108758	5.07108758
$\mathcal{O}(\varepsilon^{0})$	8.326(1)	8.3259

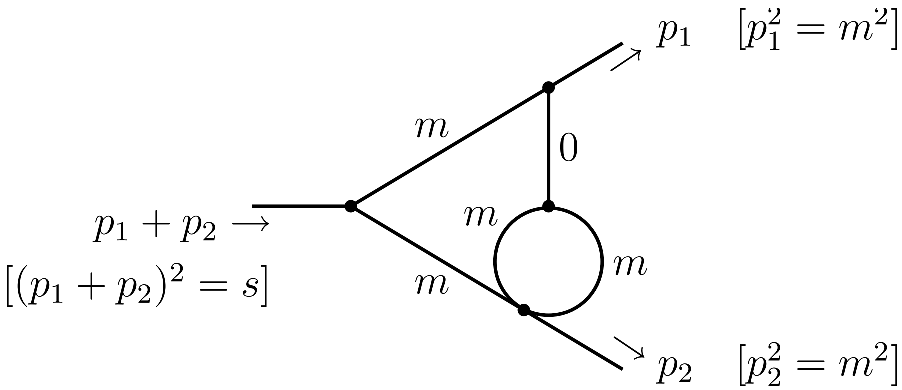
$M_{\rm Z} = 1$, $M_{\rm W} = 80/91$,
$m_{\rm t} = 180/91$

CUHRE routine,
$N = 10^6$, $\lambda = 0$ (no cuts)

*Bernstein-Tkachov method from Awramik, Czakon, Freitas, Kniehl '08

Two-loop examples

Two-loop scalar vertex diagram with soft and UV singularity:



$m = 1$, $s = 5$

	this work	analytical
$\mathcal{O}(\varepsilon^{-2})$	$-0.43040894 + 1.40496295i$	$-0.43040894 + 1.40496295i$
$\mathcal{O}(\varepsilon^{-1})$	-3.53105702	-3.53105702
$\mathcal{O}(\varepsilon^{0})$	$-1.93471(1) - 2.08763(1)i$	$-1.93471213 - 2.08762578i$

↑ using CUHRE routine, $N = 10^6$, $\lambda = 1$

↑ anal. result in terms of HPLs

Bonciani, Mastrolia, Remiddi '03

Summary

Subtraction terms useful for numerical treatment of virtual 1-/2-loop diagrams

- Similar philosophy to real corrections
- Contour deformation for diagrams with phys. cuts
- Good numerical stability, although difficulties in special cases
- Easy to automatize

Public code NICODEMOS

- Implementation into MATHEMATICA/FORTRAN code
  NICODEMOS (NUmerical Integration with COntour DEformation and MOdular Subtractions)
- Download at `http://www.pitt.edu/~afreitas/`
- Current version 1.1 (Aug. 2012): includes capabilities presented here

$\longrightarrow$ Please use and test!

Example:

```
 afreitas: t11344 > math
Mathematica 6.0 for Linux x86 (64-bit)
Copyright 1988-2007 Wolfram Research, Inc.

In[1]:= <<oneloop.m;                                            ← load package

In[2]:= gaqqden = {k1.k1, (k1-p1).(k1-p1) - mqs, (k1+p2).(k1+p2) - mqs};
                                                                ↖ define denominator...
In[3]:= gaqqnum = (2*(-4*($d-2)*(p1.p2)^2 + 4*p1.k1*(mqs*($d-1) +
     ($d-2)*p2.k1) + p1.p2*(-4*mqs*$d + (8 - 6*$d + $d^2)*k1.k1 +
     4*($d-2)*(p2.k1 - p1.k1)) + mqs*(($d-2)^2*k1.k1 + 4*($d-1)*p2.k1)))/
 (27*Pi*(mqs + ($d-2)*p1 . p2));                    ↖ ...and numerator of integrand

In[4]:= pars = {mqs,s};  momext = {p1,p2};                      ← define parameters

In[5]:= rels = {Dot[p1,p1]->mqs, Dot[p2,p2]->mqs, Dot[p1,p2]->s/2-mqs};

In[6]:= gaqqnum = SubSoft[gaqqden, gaqqnum, k1, k1];            ← subtract soft sing.

In[7]:= gaqqres  = OneLoop[gaqqden, gaqqnum, k1];               ← Feynman pars. and
                                                                  tensor reduction
In[8]:= WriteCode[gaqqres, Deform->True, WorkingDirectory->"num1"]
                                                                ↖ produce Fortran code
In[9]:= Quit
 afreitas: t11344 > num1/run1 1 5 0.5
 (0.927708096,-0.16969979) (0.000133679529,0.000133669474)      ← finite part
 (0.147820609,-0.347832796) (0.,0.)                             ← 1/ε part
 200005   0. 1  0.220965996                                     ← stats
 afreitas: t11344 > █
```

Outlook

- Work in progress:
  - Extension to 2-loop diagrams with IR divergencies in both subloops
  - Improve numerical stability in regions where denominator is small

- Instabilities for small A and large n in $\int (A - i\epsilon)^{-n}$:

Deformation

$$y_i = z_i - i\lambda z_i (1 - z_i) \frac{\partial A}{\partial z_i},$$

quadratically small when $A(\vec{z}) = 0$

$$A(\vec{y}) = A(\vec{z}) - i\lambda \sum_i z_i (1 - z_i) \left(\frac{\partial A}{\partial z_i} \right)^2 + \mathcal{O}(\lambda^2).$$

$\longrightarrow$ Alternative deformation: $y_i = z_i - i\lambda z_i (1 - z_i) \left(\frac{\partial A}{\partial z_i} \right)^{1/3}$

$\longrightarrow$ Bernstein-Tkachov method for reducing n